Influence of electron scattering on the properties of the hydrated electron

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The interest in the hydrated electron stems from its role in Chemistry, radiation damage and from the fact that it is one of the simplest quantum solutes. The ground state structure of the hydrated electron is surrounded by a major controversy. Does it form a cavity with an s-like orbital character? What is the exact value of its binding or ionization energy? Is there a long-lived surface-bound state with distinct energetics? Experimentally, these properties have been probed with photoelectron spectroscopy – for excess electrons in anion water clusters and hydrated electrons in liquid microjets. The issue with existing data is that they neglect the influence of electron scattering in the liquid on the genuine properties of the hydrated electron. As a result, the experimental binding energy is artificially high and the photoelectron angular distribution is too isotropic compared with the corresponding genuine value. This contribution takes a closer look at the effects of electron scattering on the binding energy and the orbital character (photoelectron angular distribution). A detailed electron scattering model allows the quantification of the influence of electron scattering for hydrated electrons in liquid water and in water clusters, and thus the retrieval of genuine properties from experimental data.